

# Analysis of a Lateral Field Excited Acoustic Gas Sensor Based on 128°-Rotated YX-LiNbO<sub>3</sub> Plate

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## 1. Introduction

The thickness shear mode (TSM) bulk acoustic wave (BAW) devices utilizing AT-cut quartz have been widely employed for gas and liquid sensing technology. Among them, there are two important field excitation configurations; thickness field excitation (TFE) and the lateral field excitation (LFE). Thickness field excitation implies electric field exciting a longitudinal shear motion acts along the material thickness while the lateral field excitation represents that electric field acts perpendicular to the material thickness.

To the history of BAW sensing technology, we trace back to 1959 when Sauerbrey [1] first established the Sauerbrey equation based on the linearity of the mass change on quartz surface and the frequency alternation of quartz crystal. In 1998, Vig et al.[2] proposed LFE sensors which have a larger sensitivity than TFE sensors. Recently, due to the higher coupling factor of Lithium Niobate (LiNbO<sub>3</sub>), Ma et al.[3] developed BAW sensor based on (yxl 21.82°) Lithium Niobate and found a better sensitivity to AT-cut quartz.

In this work, 128°-rotated YX LiNbO<sub>3</sub> is introduced as an alternative material of BAW gas sensors to AT-cut quartz. Both thickness field excitation (TFE) and lateral field excitation (LFE) configurations are analyzed with commercial finite element software, COMSOL Mutiphysics. The resonance behaviors, frequency responses, and sensitivities of the two thickness shear modes are then discussed.

## 2. Finite Element Analysis Model Configuration

In comparison to the finite difference and boundary element methods, the finite element method (FEM) is the most common technique especially for modeling acoustic devices due to its versatility. Therefore, 3D model of 128°-rotated YX LiNbO<sub>3</sub> BAW gas sensors are presented using the finite element software, COMSOL multiphysics.

**Figure 1** shows the geometries of TFE and LFE sensors. They have the same cross-sectional dimension of a 16 mm\*11.5 mm rectangle intersect with a circle of 16 mm in diameter and the same thickness of 269 μm. The diameter of the electrodes

is 5.75 mm. The gap which separates the semi-circular electrodes of the LFE sensor is 0.5 mm. We note that the gap is aligned to be perpendicular to the X-axis such that only one LFE mode can be excited piezoelectrically. The mode occurs at around 6.56 MHz.

## 3. Results and Discussion

### 3.1 Mesh convergence analysis

In a finite element analysis, a mesh convergence analysis should be implemented to attain a compromise between the model size and the computation run time in priority. In this section, we take the LiNbO<sub>3</sub> LFE sensor as an example. The meshes in thickness and cross section are set to be independent. The element in thickness is quadrangular. The element in cross section is triangular and its size is determined by the default mesh level in COMSOL, including coarse, normal, and fine. The resonance frequency is found to converge toward a constant of about 6.56 MHz with increasing the mesh layer in thickness and affects rarely by the mesh quality in cross section. Therefore, the mesh conditions of the 10-layer mesh in thickness and the default normal-level mesh in cross section is an acceptable compromise in the following calculations.

### 3.2 Frequency-response analysis of LiNbO<sub>3</sub> sensor

In order to understand resonance behaviors of the sensors in detail, the frequency-response is necessarily calculated. The resonance spectrum is investigated by performing a frequency-response analysis. **Figure 2** is the calculated frequency response of the 2 sensors. The displacement fields of the resonances are also included in this figure. The color represents the magnitude of the displacements. Where the resonance frequency of LiNbO<sub>3</sub> TFE is 7.50 MHz and LiNbO<sub>3</sub> LFE is 6.56 MHz.

### 3.3 Sensitivity analysis of LFE gas sensors

While the nanostructured selective film deposits on BAW sensor reacts with desired gas, the variations of electrical and mechanical property occur in the selective film. The variation range of electrical conductivity and film-gas density depends on the film material and target gas. Moreover, the film can be served as virtual electrode acting on the

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back to LFE sensor, leads to a redistribution of the exciting electric field and a significant resonance frequency shift. In this section, we investigated the resonance frequency shift of the 128° YX LiNbO<sub>3</sub> TFE and LFE gas sensor completely covered with a selective film. The poly(isobutylene) (PIB) film is taken as an calculation example of the selective film because its material parameters could be found from literature[4]. The frequency shift is computed by evaluating the resonance frequencies before and after increasing the electrical conductivity or the film-gas density of the PIB film.

The material parameters of the PIB film used in the calculation include: relative permittivity of 2.2, film density of 0.918 kg/m<sup>3</sup> and Young's modulus of 10 GPa. A 0.48 Poisson's ratio is corresponded to a rather rubbery material. The thickness of the PIB film is set to 1 μm, which is reasonable for practical deposition techniques. The continuity boundary condition is imposed at the film-substrate interface. In addition, this thickness is divided into three mesh layers to maintain a sufficient number of elements for computation accuracy. While the PIB film react with the desired gas, Young's modulus and Poisson's ratio are assumed to be invariant during gas concentration. Therefore, we adopted the FEM software to calculate the sensitivity to the variation of electrical conductivity and film-gas density of the gas sensor.

The calculation results are in **Figure 3**. The values of frequency shift are plotted with a negative sign to indicate a reduction in resonance frequency. **Figure 3(a)** shows that a gradual conductivity increase causes significant resonance frequency decreases of the both TFE and LFE gas sensors until 0.3 S/m. The frequency drop saturates finally at about -4 kHz for the TFE sensor and -1 kHz for the LFE sensor. **Figure 3(b)** shows the change of film density as a function of frequency shift to the two sensors. The LFE sensor appears a larger frequency decrease than the TFE sensor at density variation of about 4.5%.

#### 4. Conclusions

This work adopted commercial finite element software, COMSOL, to calculate the sensitivity of 128°-rotated YX LiNbO<sub>3</sub> gas sensors in LFE and TFE configuration, which operates at about 6.56 MHz. Result shows the TFE sensor has a larger sensitivity to electrical conductivity and the LFE sensor has a larger sensitivity to density variation for gas sensing. The results of this paper can provide important guidelines for designing BAW gas sensors based on LiNbO<sub>3</sub> plate.

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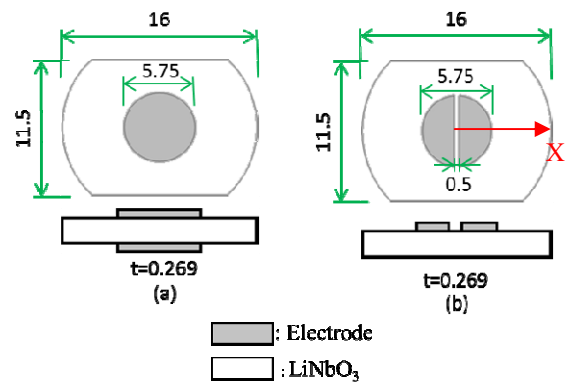


Fig. 1 Device configurations: (a) TFE and (b) LFE. (in mm)

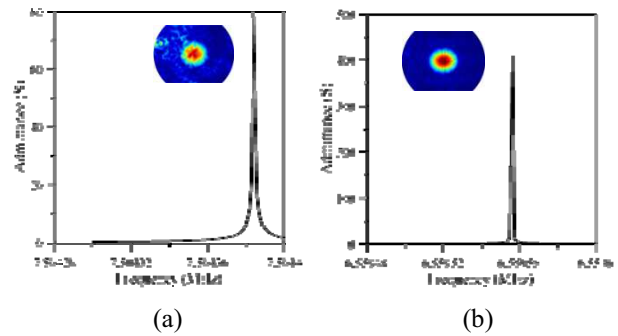


Fig. 2 Frequency responses of (a) TFE and (b) LFE sensors.

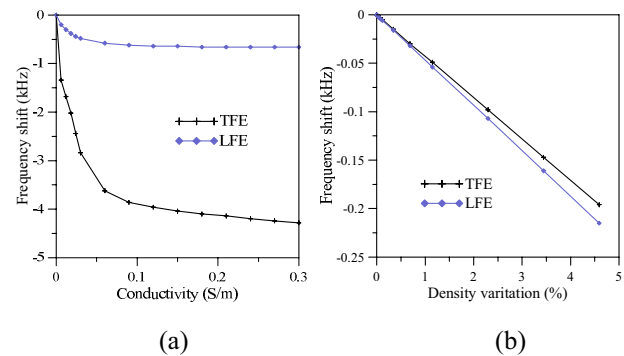


Fig. 3 Sensitivities of TFE and LFE gas sensors to (a) conductivity and (b) density variations of selective film.